REINVENT 2.0 – an AI Tool for De Novo Drug Design

Abstract

With this application note we aim to offer the community a production-ready tool for de novo design. It can be effectively applied on drug discovery projects that are striving to resolve either exploration or exploitation problems while navigating the chemical space. By releasing the code we are aiming to facilitate the research on using generative methods on drug discovery problems and to promote the collaborative efforts in this area so that it can be used as an interaction point for future scientific collaborations.